CEWES MSRC/PET TR/99-24

Contract Year Four
Programming Environment and Training (PET)
Core Support and Focused Efforts
for CEWES Major Shared Resource Center (MSRC)

July 1999

04h02499

Work funded by the DoD High Performance Computing Modernization Program CEWES Major Shared Resource Center through

Programming Environment and Training (PET)

Supported by Contract Number: DAHC94-96-C0002
Nichols Research Corporation

ERDC MSRC/PET TR/24

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Section 1: INTRODUCTION

1.1 BACKGROUND

As a result of the Annual Review for the Engineer Research and Development Center (ERDC) Major Shared Resource Center (MSRC) Programming Environment and Training (PET) program that occurred on 9-10 February 1999, a follow-on series of Core Support and Focused Efforts have been endorsed. These cover the primary Computational Technology Areas (CTAs) supported by the center and other specialty areas, including Scientific Visualization (SV), Scalable Parallel Programming (SPP) Tools, support for Historically Black Colleges and Universities (HBCUs) and Minority Institutions (MIs), Training, and Collaboration/Communication (C/C). The primary CTAs supported at ERDC MSRC are Computational Fluid Dynamics (CFD), Computational Structural Mechanics (CSM), Environmental Quality Modeling and Simulation (EQM), Climate/Weather/Oceans Modeling and Simulation (CWO), and Forces Modeling and Simulation/C4I (FMS).

The academic partners associated with ERDC MSRC PET include: the Engineering Research Center (ERC) at Mississippi State University (MSU) (Lead University); the National Center for Supercomputing Applications (NCSA) at the University of Illinois; the Center for Research in Parallel Computing (CRPC), led by Rice University and supported by the University of Tennessee, Knoxville (UTK) and the Northeast Parallel Architectures Center (NPAC) at Syracuse University; Jackson State University (HBCU Lead); Clark Atlanta University (HBCU); Ohio Supercomputing Center (OSC); Ohio State University (OSU); the Texas Institute for Computational and Applied Mathematics (TICAM) at the University of Texas at Austin; and the University of Southern California (USC).

1.2 CORE SUPPORT

"Core Support" refers to that portion of PET that captures the minimum funding required for full-time positions and university leads. Significant lead time and funding assurance are required prior to university hiring commitments, so there must be some level of assurance that annual funding will be maintained at each university throughout the program. This, of course, does not preclude corrective action based on non-performance. PET staff activities at ERDC MSRC within Core Support include, but are not limited to:

- Providing High Performance Computing (HPC) training courses for MSRC users
- Providing a continual base of academic involvement in PET
- Ensuring greater freedom in the scope of university efforts
- Providing for longer duration academic efforts

- Administration of Training and Education Facility (TEF) systems
- User outreach based on constant CTA utilization monitoring and taxonomy updates, DoD HPC User Group participation, and one-on-one user assistance as required
- Providing updated inputs to PET web pages and collaborative environments
- Regular reporting of activities/progress for each PET area
- SPP algorithm enhancement
  - Scalable parallelization fundamental issues
  - Development of **better numerics and science** for existing algorithms
- Integral PET role in computational migration
  - Support to specific key algorithm migrations as required
  - Identification of long-term algorithmic issues

The following Core Support efforts were approved for Year Four:

Nichols Research Corporation / Nichols InfoFed
- PET Leadership (Director), On-site
- PET Leadership (Academic Team Lead), On-site
- Training Coordinator, On-site
- PET Scientific Visualization Lead, On-site

Mississippi State University - ERC
- Academic Lead, Overall PET Program, Off-site
- Computational Fluid Dynamics (CFD), On-site and Off-site
- Computational Structural Mechanics (CSM), On-site

University of Illinois - NCSA
- Scientific Visualization, Off-site

Rice University - CRPC
- Scalable Parallel Programming Tools, On-site and Off-site

Syracuse University - NPAC
- Communication/Collaboration (C/C), Off-site
- Training, Off-site
- Forces Modeling and Simulation (FMS), Off-site

University of Tennessee, Knoxville
- Scalable Parallel Programming Tools, Off-site

Jackson State University
- HPC Support to HBCU/MIs, Off-site

Ohio State University
- Climate, Weather, and Ocean (CWO), On-site and Off-site

University of Texas at Austin - TICAM
- Environmental Quality Modeling (EQM), On-site and Off-site
- Computational Structural Mechanics (CSM), Off-site

1.3 FOCUSED EFFORTS

"Focused Efforts" are activities funded by the additional PET resources, which are allocated for approved "projects" based on PET team interactions with MSRC users and on proposals submitted by the university partners and approved by the PET leadership and ERDC MSRC. Focused Effort proposals are evaluated according to the following guidelines:

- Each proposed effort should be an HPC support activity related to national defense or national security.
- Relevance of proposed activity to ongoing Common HPC Software Support Initiative (CHSSI) projects is considered.
- Extent to which the proposed effort complements MSRC hardware acquisition strategy is considered.
- Proposed effort relevance to ongoing DoD Challenge Projects is considered.
- Proposed effort exploitation of the Defense Research and Engineering Network (DREN) network capabilities is considered.
- Efforts should improve the effective utilization of HPC resources via
  - Visualization and data interpretation
  - Code performance enhancements
  - Multi-architecture portability, etc.
- Proposed efforts should enhance the capability to use MSRC systems via
  - Training and graduate courses
  - HBCU/MI activities
  - Collaborative environments, etc.

Obviously, every Focused Effort cannot meet all of these criteria. These criteria are used to judge the importance of the proposed work with respect to the HPCMP mission. Focused Efforts are managed according to the following rules:

- Authority to Proceed (ATP) is based on informal proposals submitted to the PET Director and the review/concurrence of PET leadership and the government.
- Projects **must have MSRC user advocacy and participation** if at all possible.
- Projects should have specific start and end dates, schedules, work products, budgets, and periodic progress reviews (every 3-6 months).
- Each effort is managed on a project-by-project basis (i.e., funding will be allocated on this basis).

The following Focused Efforts have been approved for Year Four:

Clark Atlanta University
- Development of a Web Database (Student Internship)
- Interpretation of Large Data Sets (Data Mining) Phase I

University of Illinois - NCSA
- EQM Sci Vis Tools and Support

Ohio Supercomputer Center (OSC)
- HPC Training Courses

Rice University - CRPC
- Training Tutorial
- Fortran Pthreads Programming

University of Tennessee, Knoxville
- Parallel I/O for Distributed Applications

Syracuse University - NPAC
- Collaborative Computing Environments (Web Interfaces)
- Enforcing Scalability of Parallel Comprehensive Mine Simulator (CMS)
- HLA Integration for HPC Applications Applied to CMS
- New Directions in Distance Education and Training
- Web Interfaces for Computational Modules

Jackson State University
- Web-Based Distance Education
- Remote Scientific Visualization

University of Texas at Austin - TICAM
- General Parallel 3D Local Conservative Projection Algorithm

- Debugging, Validation, and Evolution of Parallel EQM Codes
- Adaptive Mesh Technology Applied to Damaged Structures
- Adaptive Mesh Technology for Hypervelocity Impact and Penetration Analysis

University of Southern California

- Modeling of HPC Platforms and Performance Tuning of Large Scale DoD Applications

Detailed descriptions of these Focused Efforts and Core Support Areas are provided in Section 2.

The overall working theme for ERDC MSRC is "Scalable HPC Applications and Performance." Within the context of this "umbrella," PET is supporting a number of sub-themes, including scalable computing migration, HPC training and DoD user productivity, HPC performance metrics and tools, management and interpretations of large data sets, SV of very large (terabyte scale) problems, and DoD Challenge applications. The PET Core Support and Focused Efforts support the overall ERDC MSRC theme and sub-themes.

Section 2

ERDC MSRC PET
YEAR 4 CORE SUPPORT
and
FOCUSED EFFORTS

ERDC MSRC PET YEAR 4 EFFORTS

1. **Focused Effort Title**: Development of a Web Database (Student Internship)
2. **Organization**: Clark Atlanta University
3. **Thematic Area**: HPC Training and User Productivity
4. **Lead**: Prof. R. Srikanth
5. **E-Mail Address**: srikanth@cis.cau.edu
6. **Telephone**: (404) 880-6955
7. **Fax**: (404) 880-6963
8. **Statement of Work**:

   Clark Atlanta University will provide a student to work on-site at ERDC MSRC during the months of July and August 1999. The student will help in the development of the ERDC MSRC web pages and begin to develop a database of information on all PET efforts, reports, and other information on the web site. For example, modifications to existing web structure can be made to show links from a project description page to the home pages of investigators and all the reports that resulted from that work.

   Assumption: All material and information to be supplied by ERDC MSRC.
   All material developed (web site and database) will be delivered on tape/zip medium.

9. **Deliverables:**

   - Generation of web inputs and database requirements (August 31, 1999)

1. **Focused Effort Title:** Interpretation of Large Data Sets (Data Mining) Phase I

2. **Organization:** Clark Atlanta University

4. **PI Names:** Prof. R. Srikanth and Prof. R. George

5. **Email Addresses:** srikanth@cis.cau.edu, roy@cis.cau.edu

6. **Telephone:** (404)-880-6955, (404)-880-6953

7. **Fax:** (404)-880-6963

3. **Thematic Area(s):** Management and Interpretation of Large Data Sets

8. **Statement of Work:**

In this effort CAU will examine and catalogue known structural problems of interest in CSM using several data mining (both fuzzy and crisp) techniques. The effort will produce a report that will aid in the use of data mining techniques for classes of problems of interest in CSM. Phase I will consist of the following:

Phase I:

- Running data mining algorithms (association rules, Fuzzy Rule Generator and CART) on the Taylor Impact problem.
- Benchmarking some other known problems.

Data mining is a powerful approach to provide insight into raw data. An approach used in many data mining techniques is called intentional answering. Also, soft computing is used increasingly with data mining techniques. An approach to intentional answering or data summarization utilizing soft computing methodologies is described below.

The general form of an intentional answer is QY's are F where Q is a fuzzy linguistic quantifier, Y is a class of objects and F is a property of the class or a summary that applies to the class quantified by Q. Fuzzy descriptions of linguistic quantifiers and labels help to evaluate the degree to which an intentional answer describes a given set of tuples. Bounds on such descriptions can be defined in terms of a most general specification constituent description and a most specific generalization constraint description.

One approach to data summarization is to respond to data queries with knowledge statements. An answer that incorporates knowledge statements is called an intentional answer. Intentional answering provides answers, based on domain knowledge, useful in the decision making process. An intentional answer can be extended over the same collection of facts and can be related to the extensional answer in several ways. If the extension of the intentional answer is equal to the extensional answer, then the intentional answer is perfect. If the extension of the intentional answer is contained in the

extensional answer, then the intentional answer is a constituent of the extensional answer. On the other hand, if the extension of the intentional answer contains the extensional answer, then the intentional answer is a constraint on the extensional answer. Intentional answers that do not contain facts are called pure and those that mix facts and knowledge statements are called mixed answers.

One way of deriving intentional answers consists of both classes and individual elements, in a data model that includes inheritance hierarchies. Both positive and negative terms are included in the answer. In another approach, answers are derived based on aggregate expressions. Another approach uses integrity constraints to derive purely intentional answers, while another approach uses structural constraints and rules to define entity sets that are related through generalization relations or to infer rules that express relations between values of attributes. A logic-based approach can also be employed, based on a set of first-order formulas that hold over the base predicates to derive purely intentional responses.

Both data summarization and intentional answering have the same goal -- the reduction of facts to knowledge to aid decision making. Fuzzy quantifiers, hedges, and labels are also used for data summarization. Linguistic quantifiers and linguistic hedges may be of two types viz. absolute and proportional or relative. Examples of the first type are: about 5, at least 30, exactly 3, less than 50, etc.

Absolute quantifiers specify the number of pieces of data that satisfy the summary. Examples of relative quantifiers are: more than half, most, at least 25, etc. These relative quantities are characterized by indicating the proportion of data that satisfies the summary. A relative quantity is specified as a fuzzy subset of the unit interval [0,1] whereas an absolute quantity is specified as a fuzzy subset of the set of real numbers.

Zadeh classifies hedges into Type I and Type II categories. In the case of hedges of Type I e.g., very, much, more or less, slightly, highly, etc., the hedge can be approximated by an operator acting on a single fuzzy set. In the case of hedges of Type II, e.g., technically, essentially, practically, actually, strictly, in a sense, virtually, regular, etc., the effect of the hedge is more complicated, requiring a description of the manner in which it modifies its operands.

9. Deliverables:

- Contributions to PET Annual Report
- Presentations for PET Mid-Year and Annual Reviews
- Written progress report in June 1999
- Reports of data mining results of data provided
- Investigation of other appropriate data mining tools
- Final Technical Report

ERDC MSRC PET YEAR 4 EFFORTS

1. **Core Support Area:** Scientific Visualization (SV), Off-site
2. **Organization:** University of Illinois, NCSA
3. **Lead:** Dr. Polly Baker
4. **E-Mail Address:** baker@ncsa.uiuc.edu
5. **Telephone:** (217) 244-1997
6. **Fax:** (217) 244-2909
7. **Statement of Work:**

   NCSA will provide program definition, long range planning and coordination among the PET elements that supply visualization capability. We participate in DoD-related meetings to engage in discussion with users and other MSRC personnel. We participate in national visualization meetings, to report on emerging technologies and to contribute to emerging Vis software efforts. NCSA will interact and share information with the staff of the Scientific Visualization Center and other MSRC visualization specialists. We will cover day-to-day operations, including the reporting requirements, continuing maintenance, and updating of ERDC MSRC Visualization web pages.

8. **Deliverables:**

   - Provide program direction, coordinate with national efforts such as the Alliance, NASA, DOE (ongoing)
   - Develop updated 5-year Visualization plan (July)
   - Participate in DoD-related meetings (June, November)
   - Participate in and report on national visualization meetings (August, October)
   - Presentations for PET Mid-Year and Annual Reviews
   - Maintain web site (Ongoing)
   - Written progress reports in June and December 1999
   - Participate in JSU Summer Institute (1-day, June)
   - Contributions to PET Annual Report

ERDC MSRC PET YEAR 4 EFFORTS

1. **Focused Effort Title:** EQM Sci Vis Tools and Support

2. **Organization:** University of Illinois, NCSA

3. **Thematic Area(s):** Scientific Visualization for Very Large Problems

4. **PI Name:** Dr. Polly Baker

5. **E-Mail Address:** baker@ncsa.uiuc.edu

6. **Telephone:** (217) 244-1997

7. **Fax:** (217) 244-2909

8. **Statement of Work:**

   NCSA will complete the current application-specific work supporting EQM and migrate the capabilities developed here to a solution that is compatible with collaborative visualization

9. **Deliverables:**

   - Complete all image and movie sequences (May)
   - Combine CbayVisGen and Transport Flux Visualization tools (November)
   - Deliver documentation for CbayVisGen/Transport Flux tool (July)
   - Explore and implement strategies for supporting collaborative visualization (December)
   - Transfer collaborative visualization tool (January)
   - Presentations for PET Mid-Year and Annual Reviews
   - Written progress reports in June and December 1999
   - Contributions to PET Annual Report
   - Final Technical Report

ERDC MSRC PET YEAR 4 EFFORTS

1. **Core Support Area:** HPC Support to HBCU / MIs, Off-site
2. **Organization:** Jackson State University
3. **Lead:** Prof. Willie G. Brown
4. **E-Mail Address:** wbrown@jsums.edu
5. **Telephone:** 601-974-6170
6. **Fax:** 601-974-6171
7. **Statement of Work:**

   Jackson State University (JSU) will provide a core level of effort to support student training activities at JSU. This will include HBCU/MI web page maintenance and updating, HBCU/MI capabilities database, users group meetings, visits to ERDC MSRC, and conduct of the Summer Institute.

8. **Deliverables:**

   - HBCU/MI web pages
   - HPC Summer Institute
   - Contributions to PET Annual Report
   - Written progress reports in June and December 1999
   - Presentations for PET Mid-Year and Annual Reviews
   - Attendance and Participation in PET meetings, conferences, workshops, colloquia, etc.

ERDC MSRC PET YEAR 4 EFFORTS

1. **Focused Effort Title:** Web-Based Distance Education
2. **Organization:** Jackson State University
3. **Thematic Area(s):** HPC Training and DoD User Productivity
4. **PI Name:** Prof. Willie G. Brown, Prof. Debasis Mitra, Prof. Q. Malluhi
5. **E-Mail Address:** wbrown@jsums.edu**,** dmitra@jsums.edu, qmalluhi@jsums.edu
6. **Telephone:** 601-974-6170
7. **Fax:** 601-974-6171
8. **Statement of Work:**

   During Year 4, JSU proposes to continue the ERDC MSRC web-based distance learning collaboration with Syracuse University. Based on lessons learned in previous years, the Tango software has been revised and improved. JSU and Syracuse University will use the new version for course delivery during the fall 1999 and spring 2000 semesters. JSU and Syracuse University will extend the partnership to include students at other HBCU/MIs, as well as DoD users at MSRCs and Distributed Centers. Specifically, instructors at Syracuse University will deliver one graduate level course to JSU and two other HBCU/MIs, e.g., Clark Atlanta University and Morgan State University during the Fall 1999 and Spring 2000 semesters. In addition, instructors at JSU will deliver one undergraduate course to a select group of HBCU/MIs including, but not limited to, Alcorn State University and Mississippi Valley State University. All courses will be made available to DoD personnel at the ERDC MSRC.

9. **Deliverables:**

   - Fall 1999 and spring 2000 semesters: Graduate Course in HPC, delivered by NPAC to JSU, two other HBCU/MIs, and the ERDC MSRC
   - Fall 1999 and Spring 2000 semesters: Undergraduate Course in HPC, delivered by JSU to Alcorn State University and Mississippi Valley State University
   - Evaluation, Results, Lessons Learned from all courses
   - Final Technical Report
   - Written progress reports in June and December 1999
   - Presentations for PET Mid-Year and Annual Reviews
   - Contributions to PET Annual Report

ERDC MSRC PET YEAR 4 EFFORTS

1. **Focused Effort Title:** Remote Scientific Visualization
2. **Organization:** Jackson State University
3. **Thematic Area(s):** Scientific Visualization
4. **PI Name:** Prof. Willie G. Brown
5. **E-Mail Address:** wbrown@jsums.edu
6. **Telephone:** 601-974-6170
7. **Fax:** 601-974-6171
8. **Statement of Work**

JSU proposes to continue its support of the ERDC MSRC in the area of scientific visualization. This activity will include sustained development of remote scientific visualization technologies and tools.

In order for the Major Shared Resource Center (MSRC) concept to succeed, on the scale intended, several major problems must be overcome. One of these problems is high performance distributed data storage and retrieval, i.e., the ability for geographically distributed users to efficiently and simultaneously access large amounts of data that are also stored in geographically distributed sites. This is an area in which JSU has considerable expertise. Remote scientific visualization is, in many ways, a subproblem, or application problem, of high performance distributed data storage and retrieval. We will continue with efforts to develop and deploy architectures and tools that allow DoD users at distributed sites to create and access renderings of scientific data, remotely and simultaneously. We will concentrate on developing a generic workstation client, with a graphical user interface, that enables users to manipulate visualizations in a distributed, collaborative environment. JSU has been working with Syracuse University (SU) to deliver distance education via the Tango system, which is an instantiation of the kind of environment just described. We will take advantage of this experience and strengthen the JSU/SU/ERDC MSRC relationship by visiting the Tango group at SU at least once during Year 4. This will ensure that the remote visualization client will interface with Tango. The client will be adaptable to various platforms such as SGI, PC, Panoram, CAVE, Immersadesk, etc. We will acquire appropriate data and produce at least one visualization during year 4.

In addition, we will deliver at least two workshops/demonstrations on remote scientific visualization. These will be presented as part of a bi-monthly Tango/web-based HPC seminar series to be hosted by JSU.

9. Deliverables:

- Prototype remote scientific visualization client
- At least one visit by a JSU researcher to Syracuse University's Tango group
- At least one scientific visualization
- At least two (2) workshops/demonstrations (dates and time to be determined) covering remote scientific visualization
- Written progress reports in June and December 1999
- Presentations for PET Mid-Year and Annual Reviews
- Contributions to PET Annual Report

ERDC MSRC PET YEAR 4 EFFORTS

1. **Core Support Area:** Academic Lead, Overall PET Program, Off-site
2. **Organization:** Mississippi State University, ERC
3. **Lead:** Prof. Joe Thompson
4. **E-Mail Address:** joe@erc.msstate.edu
5. **Telephone:** (601) 325-7299
6. **Fax:** (601) 325-7692
7. **Statement of Work:**

   MSU-ERC will provide a core level of effort to support the academic leadership of the PET program at ERDC MSRC. Responsibilities include, but are not limited to, participation the Academic Executive Committee (ExComm) for PET across the four MSRCs; maintaining knowledge of current status of all Focused Efforts ongoing at the (currently) ten participating university partners; review and recommendations for funding of PET Focused Efforts and participation in planning and execution of PET meetings (Mid-Year Review, Annual Review, workshops, DoD Users Meeting, etc.) as appropriate. MSU-ERC will select and attend conferences and other meetings that have high payoff and direct application for the PET Program.

8. **Deliverables:**

   - Trip reports for conferences and user contacts (as conducted)
   - Support for JSU Summer Institute
   - Contributions to PET Annual Report
   - Written progress reports in June and December 1999

ERDC MSRC PET YEAR 4 EFFORTS

1. **Core Support Area:** Computational Fluid Dynamics (CFD), On-site and Off-site
2. **Organization:** Mississippi State University, ERC
3. **Lead:** Prof. Bharat Soni
4. **E-Mail Address:** bsoni@erc.msstate.edu
5. **Telephone:** (601) 325-2647
6. **Fax:** (601) 325-7692
7. **Statement of Work:**

   MSU-ERC will provide a core level of effort to support the CFD on-site position for the PET program at ERDC MSRC. MSU will provide a core level of effort to support technology transfer, user outreach, training and assessment of targeted codes and algorithms in CFD. Targeted codes include, but are not limited to, the CFD CHSSI codes, CH3D, RMA10, etc. Technology of interest includes, but is not limited to, grid generation codes, parallelization of CFD algorithms, numerical solvers, management and interpretation of large data sets, adaptive and meshless techniques, etc. MSU will maintain frequent contact with the DoD CTA Lead for CFD. MSU will select and attend focused conferences and other meetings that have high payoff and direct application for user interaction and technology transfer.

8. **Deliverables:**

   - Trip reports for conferences and user contacts (as conducted)
   - Presentations for PET Mid-Year and Annual Reviews
   - Contributions to PET website for CFD as appropriate
   - Contributions to PET Annual Report
   - Written progress reports in June and December 1999
   - CFD Training Course
   - JSU Summer Institute
   - At least one technical report submitted by on-site lead

ERDC MSRC PET YEAR 4 EFFORTS

1. **Core Support Area:** Computational Structural Mechanics (CSM), On-site

2. **Organization:** Mississippi State University, ERC

3. **Lead:** Prof. Joe Thompson

4. **E-Mail Address:** joe@erc.msstate.edu

5. **Telephone:** (601) 325-7299

6. **Fax:** (601) 325-7692

7. **Statement of Work:**

   MSU-ERC will provide a core level of effort to support the CSM on-site position for the PET program at ERDC MSRC. MSU will provide a core level of effort to support technology transfer, user outreach, training and assessment of targeted codes and algorithms in CSM. Targeted codes include, but are not limited to, EPIC, CTH, DYNA3D, and NASTRAN. Technology of interest includes, but is not limited to, grid generation codes, management and interpretation of large (terascale) data sets, adaptive and meshless techniques, etc. MSU will maintain frequent contact with the DoD CTA Lead for CSM to understand the priorities and ongoing CHSSI activities. MSU will select and attend focused conferences and other meetings that have high payoff and direct application for user interaction and technology transfer. MSU will provide on-site support for CSM related activities in large data sets and scientific visualization at Clark Atlanta, NCSA, and MSU.

8. **Deliverables:**

   - Trip reports for conferences and user contacts (as conducted)
   - Presentations for PET Mid-Year and Annual Reviews
   - Contributions to PET website for CSM as appropriate
   - Written progress reports in June and December 1999
   - Contributions to PET Annual Report
   - At least one technical report submitted by on-site lead

ERDC MSRC PET YEAR 4 EFFORTS

1. **Core Support Area:** Climate, Weather and Ocean (CWO), On-site and Off-site
2. **Organization:** Ohio State University
3. **Lead:** Prof. K. Bedford, Dr. P. Sadayappan
4. **E-Mail Address:** bedford.1@osu.edu, sadayappan.1@osu.edu
5. **Telephone:** (614) 292-7338, (614) 292-0053
6. **Fax:** (614) 292-3780
7. **Statement of Work:**

   OSU will provide a core level of effort to support technology transfer, user outreach, training, and assessment of targeted codes and algorithms in CWO. Targeted codes include, but are not limited to, WAM, CH3D, SWAN, SED, FRM, MMS, and COSED. Technologies of interest include, but are not limited to, application of circulation and wave models to sea condition prediction; coupling of wave, sediment and circulation models, etc. OSU will maintain frequent contact with the DoD CTA Lead for CWO to understand the priorities and ongoing CHSSI activities, as well as with the local CWO representative at ERDC MSRC. OSU will select and attend focused conferences and other meetings that have high payoff and direct application for use interaction and technology transfer. Targeted training includes, but is not limited to, participation in the JSU Summer Institute and presentation of two courses.

8. **Deliverables:**

   - Web page updates
   - Trip Reports
   - Presentations for PET Mid-Year and Annual Reviews
   - DoD HPCMP Users Group Meeting
   - Supercomputing ’99 Presentation
   - JSU Summer Institute
   - Mesoscale Atmospheric Modeling Workshop
   - Parallelization Training Course
   - Completion of SWAN sub-nest in WAM
   - Written progress reports in June and December 1999
   - Contributions to PET Annual Report
   - At least one technical report submitted by on-site lead

1. **Focused Effort Title:** HPC Training Courses
2. **Organization:** Ohio Supercomputer Center (OSC)
3. **Thematic Area(s):** HPC Training and DoD User Productivity
4. **Lead:** Dr. Richard Pritchard, Leslie Southern, Ken Flurchick
5. **E-Mail Address:** rhp@osc.edu, leslie@osc.edu, kenf@osc.edu
6. **Telephone:** (614) 292-1163, (614) 292-9248, (614) 292-9248
7. **Fax:** (614) 292-7168
8. **Statement of Work:**

OSC will teach the following three courses of interest to the HPC community:

Using the CRAY T3E for Code Development and Analysis
Length: 2 days
Description: This course covers a range of hardware and software features available to users of the CRAY T3E. The topics covered include hardware, operating system, interactive usage, process management, environment management, batch processing, compilers, debugging tools, performance analysis tools, timing routines, single-node numerical libraries, parallel numerical libraries, fine-grained parallelism, data locality, and streams.

Using the SGI Origin2000 for Code Development and Analysis
Length: 3 days
Description: This "hands-on" course covers an extensive range of hardware and software features available to users of the SGI Origin2000(O2K). The topics covered are:

- Introduction to the O2K
- The MIPS R10000 Processor
- The Architecture of the O2K
- An Introduction to the IRIX operating system
- Programming Environment
- Compiling Systems (including "useful" options)
- Batch processing
- Single-Processor Performance Analysis tools
- OpenMP Parallel Programming
- SGI Data Distribution Directives
- Automatic Parallelization
- Message Passing Libraries for Parallel Programming
- Debugging Tools

The format of the course will consist of lectures on these topics as well as lab sessions in which participants will write their own parallel code and run software tools.

How to use Parallel Linear Algebra Library Routines
Length: 2 days
Description Specifically, this advanced course will focus on the libraries which have become the "de facto" standards for parallel linear algebra: SCALAPACK (the parallel successor to LAPACK) and PBLAS (the parallel successor to BLAS). Both of the libraries build upon calls to the BLACS library which will set up the processors in a communication grid that matches the problem being solved and distributes appropriate array elements to the correct processor's memory to achieve good performance.

9. Deliverables:

- Course material for each course
- Written progress reports in June and December 1999
- Presentations for PET Mid-Year and Annual Reviews
- Contributions to PET Annual Report

ERDC MSRC PET YEAR 4 EFFORTS

1. **Core Support Area:** Scalable Parallel Programming Tools, On-site and Off-site

2. **Organization:** Rice University, CRPC

3. **Lead:** Prof. Richard Hanson

4. **E-Mail Address:** koolhans@cs.rice.edu

5. **Telephone:** 713-285-5304

6. **Fax:** 713-285-5136

7. **Statement of Work:**

   Rice will provide support in the general areas of technology transfer, user and community outreach, and training in new technologies related to SPP tools. The tools include parallel debugging tools, parallel application development software libraries, and access to expertise in key areas of importance to ERDC MSRC and its DoD users. Rice will coordinate tools activities by the PET team at Rice and University of Tennessee, Knoxville, and provide on-site tools support. Rice researchers will work with the Rice on-site person to engage users, provide technology transfer, and focus on ERDC MSRC needs. Rice personnel will attend related meetings and conferences that support the ERDC MSRC mission. For each such trip Rice will submit, in advance, a rationale to allow NRC management to determine the coverage of ERDC MSRC PET funds for the related expenses.

   Work will proceed on parallelization efforts for the SWAN and STWAVE codes. The nature of the work will be analysis of integrators, use of parallel solvers, and the use of MPI, OpenMP, or Pthreads as appropriate for achieving high performance. Training (tutorials and seminars) will be conducted at ERDC MSRC and elsewhere as needed for appropriate tools and/or parallel programming topics.

8. **Deliverables:**

   - Trip Reports for Conferences and User Contacts
   - Contributions to PET Annual Report
   - Presentations for PET Mid-Year and Annual Reviews
   - Written progress reports in June and December 1999
   - Support to JSU Summer Institute
   - At least one technical report submitted by on-site lead

ERDC MSRC PET YEAR 4 EFFORTS

1. **Focused Effort Title:** Training Tutorial
2. **Organization:** Rice University, CRPC
3. **Thematic Area(s):** HPC Training and DoD User Productivity
4. **PI Name:** Prof. Richard Hanson
5. **E-Mail Address:** koolhans@cs.rice.edu
6. **Telephone:** 713-285-5304
7. **Fax:** 713-285-5136
8. **Statement of Work:**

   Rice University will conduct a tutorial at Rice on concurrent programming with POSIX threads (Pthreads). Emphasis will be placed on a core set of Pthread functions that are thought to be the most useful for scientific computations. Basic principles of concurrent programming will be presented along with examples that illustrate the potential pitfalls and complications that may be encountered. This course will be relevant to programmers of shared-memory or SMP architectures.

9. **Deliverables:**

   - Tutorial Class
   - Contributions to PET Annual Report
   - Presentations for PET Mid-Year and Annual Reviews

1. **Focused Effort Title**: Fortran Pthreads Programming
2. **Organization:** Rice University, CRPC
3. **Thematic Area:** Scalable Computing Migration
4. **Pi Names:** Prof. Richard Hanson
5. **Email:** koolhans@cs.rice.edu
6. **Telephone:** 713 285 5304
7. **Fax:** 713 285 5136
8. **Statement Of Work:**

It is now understood that thread models for parallel programming can be effective to achieve high-performance. Threads are a shared-memory programming model and are particularly important for programming machines containing computational nodes that combine two or more CPUs sharing a single address space on the node. We believe that threaded programs provide one of three basic successful techniques for parallelism. (Other primary techniques are message passing and tuple spaces.)

When an application programmer wants to use the POSIX threads (Pthreads) standard library, it is currently necessary to use C, since no standard currently exists for Fortran. Nevertheless, many legacy codes exist in Fortran that cannot be conveniently converted to C. The theme of this proposed foundation work is therefore "making Pthreads usable by the DoD MSRC programmer, in Fortran." Major plans for the project are:

- We will create a comprehensive validation and verification suite for the Fortran 90 Pthreads API. This test suite will initially be implemented on the shared-memory SGI Origin2000 platform since the API was originally developed on this platform. It is expected that the test suite will be transportable to other architectures onto which the API will be ported.

- We will prepare a significant journal article and pre-print for a Fortran 90 programmer's interface to Pthreads. An established version of this work is available for the C programmer in the form of Posix threads. On-site personnel at ERDC MSRC have drafted a Fortran 90 interface to the IEEE Posix 1003.1c standard. Plans are to submit the paper and the package to a panel of interested reviewers from industry for comments on design and implementation of the API. These comments will be incorporated into the journal article, as appropriate, and submitted to a suitable journal, probably ACM-TOMS, for publication.

- We will pursue an aggressive transfer of Pthreads programming skills to MSRC users, researchers, and code developers with training and consultation efforts.

9. Deliverables:

- Provide a tutorial on concurrent programming with Pthreads at ERDC MSRC (Completion date: July 1999)
- Write a comprehensive test and validation package for the Fortran 90 API for Pthreads on the SGI Origin2000 (Completion date: October 1999)
- Port the test package to the SUN Enterprise and IBM SP3 platforms and any other multiple-CPU hardware for which the Fortran 90 Pthreads API has been installed (Completion date: November 1999)
- Write up documentation describing the design and implementation of the Fortran 90 API and the test suite for comment from interested parties (Completion date: November 1999)
- Revise API code and test suite based on comments (Completion date: January 2000)
- Provide source code for distribution of the F90 API (Completion date: March 2000).
- Document this effort in a ERDC MSRC report - This document shall also be considered for journal publication (Completion date: March 2000)
- Written progress report in December 1999
- Presentations for PET Mid-Year and Annual Reviews

1. **Focused Effort Title:** Modeling of HPC Platforms and Performance Tuning of Large Scale DoD Applications

2. **Organization:** University of Southern California

3. **Thematic Area(s):** Scalable Computing Migration, HPC Performance Metrics and Tools

4. **PI Name:** Prof. Viktor K. Prasanna

5. **E-Mail Address:** prasanna@usc.edu

6. **Telephone:** (213) 740-4483

7. **Fax:** (213) 740-4418

8. **Statement of Work:**

Many HPC platforms have been introduced with various architectural and software features. In Phase 1 of our current focused effort, we have studied low level hardware benchmarks to understand the performance of these features. We developed a uniform framework for evaluating the performance of various HPC platforms (such as IBM SP, Cray T3E, and SGI Origin2000). The main objective was to define, and through experimentation, determine a set of meaningful parameters to evaluate the performance of state-of-the-art HPC platforms for stressing DoD applications. In Phase 2 of our current focused effort, we are extending our work in Phase 1 to define a model of HPC platforms that can be employed by end-users to predict the performance of various algorithms. This model has been designated the Integrated Memory Hierarchy (IMH) Model. It will model the computation/communication cost at the various levels of the memory hierarchy, including cache, main memory, remote memory and secondary storage.

9. **Deliverables:**

- Research report on memory hierarchy data access optimization: August 1999 (An abstract of this manuscript will be submitted to SC99)
- Optimized code for demonstrating the use of the IMH model and the proposed methodology for developing large scale DoD applications: October 31, 1999
- Report on the analysis and benchmarking of CSM applications
- Final Technical Report
- Written progress reports in June and December 1999
- Contributions to PET Annual Report
- Presentations for PET Mid-Year and Annual Reviews

1. **Core Support Area:** Communication/Collaboration (C/C), Off-site
2. **Organization:** Syracuse University, NPAC
3. **Lead:** Dr. David Bernholdt
4. **E-Mail Address:** bernhold@npac.syr.edu
5. **Telephone:** 315-443-3857
6. **Fax:** 315-443-1973

7. **Statement of Work:**

Syracuse will provide a core level of effort to support technology transfer, user outreach, training, and assessment of tools and technologies to facilitate communication and collaboration among the PET team and users of the ERDC MSRC. Technologies of interest include, but are not limited to, both synchronous and asynchronous collaboration over the Internet and use of databases to manage large volumes of information, especially when coupled with web servers to facilitate access to the information. Syracuse will provide an appropriate level of effort to support the deployment and use of the Tango collaboratory tool, emphasizing robustness and core collaboration functionality. Syracuse will continue to operate and enhance web-linked database applications it has developed for ERDC MSRC, and, as requested, assist with transfer to on-site computer systems. Syracuse will maintain frequent contact with ERDC MSRC Webmaster, database administrators, and other on-site personnel to insure that C/C resources provide the maximum utility to the PET/user community. Syracuse will also maintain regular contact with PET team members to assess needs. Syracuse will select and attend focused conferences and other meetings that have high payoff and direct application for team and user interaction and technology transfer.

Targeted Codes/Algorithms:

The primary focus of our work on C/C is on the TANGO Interactive collaboratory system. With support from the ERDC MSRC PET program as well as the other MSRCs and outside organizations, we have made excellent progress in terms of the functionality and robustness of Tango in the last several years. With the basic system in good shape, we now wish to focus our PET-supported efforts on enhancements, which are important to use of the system within DoD.

1) Addressing security concerns
2) An “out-of-browser” version of Tango to provide an alternative to the problems inherent in the current tight browser integration of the system.
3) Support for the interactions inherent in a formal meeting or briefing.

Training:

We plan to offer a tutorial session on the TANGO Interactive system, covering collaboration, integration of HPC applications into the Tango collaborative environment, etc. This training will be preceded by a "Tango Open House" to give MSRC, PET, and DoD staff a chance to see and try out TANGO in a variety of different collaborative applications.

8. Deliverables:

- Trip reports for conferences and user contacts (as appropriate)
- Contributions to PET Annual Report
- Contribute materials pertaining to collaboration and communication technologies to the ERDC MRSC PET C/C web site (on-going)
- Report on asynchronous collaboration tools and their possible roles within the ERDC MSRC and PET organizations
- TANGO Tutorial and Open House at ERDC MSRC (to be determined)
- Development of a domain-specific search engine in Climate, Weather and Ocean Modeling (CWO), in collaboration with the PET CWO group (initial version August 1999 with on-going support and enhancement)
- On-going operation and enhancement of web-linked database applications
- Enhanced security support for TANGO Interactive (in stages: July 1999, November 1999, March 2000)
- Out-of-browser version of TANGO Interactive (prototype September 1999, production March 2000)
- Written progress reports in June and December 1999
- Presentations for PET Mid-Year and Annual Reviews

ERDC MSRC PET YEAR 4 EFFORTS

1. **Core Support Area:** Training, Off-Site
2. **Organization:** Syracuse University, NPAC
3. **Lead:** Dr. David Bernholdt
4. **E-Mail Address:** bernhold@npac.syr.edu
5. **Telephone:** 315-443-3857
6. **Fax:** 315-443-1973
7. **Statement of Work:**

Syracuse will provide a core level of effort to support technology transfer, user outreach, and long-range leadership on issues of technology, tools, and techniques related to PET Training and Educational needs. Technologies of interest include, but are not limited to, synchronous and asynchronous web/Internet-based distance education tools, electronic repositories of training materials, etc. Of particular, but not exclusive, interest are the Tango and WebWisdom systems developed by Syracuse. Syracuse will provide an appropriate level of effort to support these tools, as they are used in a variety of PET-supported educational and training projects, emphasizing the general robustness of the tools. Syracuse will maintain frequent contact with the on-site Training team at the ERDC MSRC to understand the needs and use of training technology at the MSRC. Syracuse will also be active in meetings of the PET Program-Wide Training Group, especially in monitoring and advising on the program-wide deployment of tools and technologies. Syracuse will select and attend focused conferences and other meetings that have high payoff and contribute directly to providing leadership on training technology issues.

Training:

As part of our effort to support the use of distance training tools within the PET program, we plan to offer a Distance Training Workshop covering approaches for both synchronous and asynchronous modes of delivery. We expect to emphasize TANGO Interactive as the primary tool for synchronous delivery and WebCT as a framework for asynchronous training. This workshop is meant both to support those groups who have already committed to provide a Tango-based distance training during Year 4, but also to adopt distance training.

8. **Deliverables:**

- Trip reports for conferences and user contacts (as appropriate)
- Contributions to PET Annual Report
- Contribute materials pertaining to education and training technologies to the ERDC MRSC PET Training web site

- Involvement in PET Program-Wide Training Group meetings and activities
- Ongoing support and enhancement of TANGO Interactive and WebWisdom NT in support of education and training activities
- Written progress reports in June and December 1999
- Presentations for PET Mid-Year and Annual Reviews
- Distance Training class
- Distance Education at JSU

1. **Core Support Area:** Forces Modeling and Simulation (FMS), Off-site
2. **Organization:** Syracuse University, NPAC
3. **Lead:** Dr. David Bernholdt
4. **E-Mail Address:** bernhold@npac.syr.edu
5. **Telephone:** 315-443-3857
6. **Fax:** 315-443-1973

7. **Statement of Work:**

In Year 4, we propose to continue the technology tracking activities and web page development to support further evolution of WebHLA. We also propose to develop a set of tutorials and training materials on porting existing simulations to HLA-compliant HPC modules with Web/Commodity interfaces using WebHLA platforms. In Year 3, we made significant progress with bringing our WebHLA concepts and early prototypes to first distributed demonstrations of relevance for the DoD Modeling and Simulation community and the DoD High Performance Computing community such as our Parallel CMS (Comprehensive Mine Simulator), successfully demonstrated in the HPCMO booth at SC98 in Orlando, FL. Bob Wasilausky, the FMS CTA Lead said after the demo that he was impressed with both the quality and quantity of our work and he encouraged us to continue to pursue and our roadmap towards WebHLA defined as the integration point of Web/Commodity, HPC and HLA technologies in support of the FMS users and applications.

Training

Our training materials will be based on lessons learned in our Parallel CMS work and will cover the following components:

- ModSAF for vehicle and terrain modeling (by STRICOM)
- Mak Stealth for battlefield visualization (by Mak Technologies)
- Comprehensive Mine Simulator by Ft Belvoir, NightVision and Electronic Sensors Directorate
- DirectX/Direct3D based NT battlefield viewer
- JWORB (Java Web Object Request Broker)
- Object Web TRI; i.e., Java/CORBA based implementation of DMSO RTI 1.3 as a JWORB service
- C++ interface library that allows wrapping a C++ simulation code as an HLA CORBA object, linkable to OW-RTI
- WebFlow for visual-authoring web based distributed dataflow applications
- OMBuilder FEDEP tools for visual authoring HLA compliant FOMs (Federation Object Models) and SOMs (Simulation Object Models)

As the HLA user community systematically grows in response to the DoD-wide mandate for all simulations to comply with HLA by year 2001, we feel that WebHLA training will be useful for several high performance simulation groups and projects within the DoD HPC Modernization Program.

8. Deliverables:

- A set of training materials, accessible in various formats, including
  - Web pages
  - Presentations (September 1999)
  - Documentation (December 1999)
  - Real-time interactive, WebHLA based distance training (March 2000)
- Trip Reports
- Scientific papers and presentations derived from ERDC MSRC PET supported activities (as available)
- Development and support of the ERDC MSRC FMS webspace and the extensive FMS webspace hosted at NPAC (ongoing)
- Technology tracking report (March 2000 and other times as appropriate)
- Contributions to PET Annual Report
- Written progress reports in June and December 1999
- Presentations for PET Mid-Year and Annual Reviews
- Support to the JSU Summer Institute.

ERDC MSRC PET YEAR 4 EFFORTS

1. **Focused Effort Title:** Collaborative Computing Environments (Web Interfaces)
2. **Organization:** Syracuse University, NPAC
3. **Thematic Area(s):** HPC Training and DoD User Productivity
4. **PI Name:** Dr. David Bernholdt
5. **E-Mail Address:** bernhold@npac.syr.edu
6. **Telephone:** 315-443-3857
7. **Fax:** 315-442-1973
8. **Statement of Work:**

In this project, we will develop prototype collaborative research environments through the integration of HPC applications with the Tango, combining the efforts of our "Web Interfaces" group with those of our Collaboration (Tango) group. Applications will be drawn from those we have worked with on our "web interfaces" efforts (a Year 3 project which has spawned two Year 4 project proposals, and is related to the ASC "Gateway" project now getting underway). This is the most natural application pool to work with initially, because we are already familiar with their user interface and operation. Since every application presents a unique mix of issues with respect to "collaboratization", we will choose for our demonstration prototypes applications which can be treated as a fairly general model for certain aspects of the collaboratization problem—for example, the sharing of a Java-based GUI or sharing of a graphical post-processing tool. The latter is an especially complex problem in general, but building on NCSA and NPAC experience in shared visualization, we will evaluate the possibility of including this in our prototype applications.

Cooperative use of large, complex HPC applications for purposes of research or education can be quite cumbersome. Quite often, the only practical solution is that collaborators must sit down together in the same room in order to effectively work together with such systems. However, the emergence of flexible electronic collaboration frameworks offers the potential to remove this bottleneck. Tango Interactive is an example of a simple, open collaborative framework with published APIs and straightforward protocols, which can be used to connect a wide variety of applications, including HPC applications. Tango-connected HPC applications would then become part of the collaborative environment offered by Tango, which already includes a wealth of essential tools for basic collaboration and education (including a shared text editor, shared telnet/terminal emulator, and other capabilities required for technical collaboration).

9. Deliverables:

- Selection of first prototype application (August 1999)
- "Beta" release of first collaborative HPC application delivered for testing and feedback (October 1999)
- Final version of first collaborative HPC application delivered (March 2000)
- Selection of second prototype application (October 1999)
- Release of second collaborative HPC application for testing and feedback (March 2000)
- Module on interfacing HPC applications to Tango to be delivered as part of planned Tango Tutorial (C/C Core)
- Final Technical Report
- Written progress reports in June and December 1999
- Presentations for PET Mid-Year and Annual Reviews
- Contributions to PET Annual Report

1. **Focused Effort Title:** Enforcing Scalability of Parallel Comprehensive Mine Simulator (CMS)

2. **Organization:** Syracuse University, NPAC

4. **PI Name:** Dr. David Bernholdt

5. **E-Mail Address:** bernhold@npac.syr.edu

6. **Telephone:** 315-443-3857

7. **Fax:** 315-443-1973

3. **Thematic Area(s):** Scalable Computing Migration

8. **Statement of Work:**

We proposed to develop a fully scalable production quality Parallel CMS module as a Year 4 Focused Effort. Apart from experimenting with and selecting the optimal configuration of compiler programs, we will also explore other parallelization techniques based on MPI, CRAY SHMEM, OpenMP and SPEEDES communication models. Both ERDC and ARL MSRCs have supported aspects of CMS parallelization over the last few years. In Year 3, we made major progress in this project: we ported the CMS code to the SGI Origin2000 platforms at ERDC MSRC and ARL MSRCs and we were also running our Parallel CMS on the SGI Origin2000 provided by the ASC MSRC for the HPCMO booth at Supercomputing '98 in Orlando, FL, November 1998. After performing the port, we conducted tests to accumulate timing results and evaluate efficiency of our parallel implementation. Performance results we got indicated that our parallel port offered almost linear speedup, i.e., perfect scalability up to and including 4 processors, but the performance deteriorates for 8 or more processors. In a sequence of crosschecks, we identified the reason as related to rather complex object-oriented data structures (including dynamic linked lists of irregular objects), present in the inner loop of the C++ CMS code. We performed some modifications of the code, simplifying the inner simulation loop, but we learned in the meantime from Ft. Belvoir that their latest version of CMS performs several additional computations in the inner loop (such as continuous thermal computations for all mines, associated with the new environmental simulation support) that need to be taken into account in our analysis and parallelization process. Hence, to turn our prototype Parallel CMS into a more robust and scalable parallel module, we need to go more deeply into the CMS code and perform a significant reorganization of the innerloop.

9. **Deliverables:**

- Parallel CMS module, scalable over the processor range on SGI Origin2000 (preliminary September 1999, Final March 2000)

- Analysis of performance and tradeoffs between various communication modes (Preliminary September 1999, Final March 2000)
- Installation of the scalable Parallel CMS module at ERDC and ARL MSRCs (March 2000)
- Evaluation of total CPU power for Metacomputing CMS on multi-MSRC platform. (Preliminary September 1999, Final March 2000)
- Final Technical Report
- Written progress reports in June and December 1999
- Presentations for PET Mid-Year and Annual Reviews
- Contributions to PET Annual Report.

1. **Focused Effort Title:** HLA Integration for HPC Applications Applied to CMS
2. **Organization:** Syracuse University, NPAC
3. **Thematic Area(s):** Scalable Computing Migration
4. **PI Name:** Dr. David Bernholdt
5. **E-Mail Address:** bernhold@npac.syr.edu
6. **Telephone:** 315-443-3857
7. **Fax:** 315-443-1973
8. **Statement of Work:**

In this proposal we will address two related goals. First, the need for message passing based coarse grain parallelism for CMS and second, integration of classic HPC applications into FMS simulations. The latter is essentially equivalent to HLA compliant versions of these applications. Both goals can be elegantly addressed by using a computing environment built around distributed (or meta) computing built on top of HLA.

From the parallel architecture point of view, this project will develop a distributed memory version of CMS which can then be ported to distributed memory MPPs such as the IBM SP. From the metacomputing management point of view, this task develops and tests tools for runtime management of distributed resources, initially prototyped in a controlled commodity cluster environment, and in the next stage to be expanded to a multi-MSRC metacomputing platform. Finally, from the parallel hardware availability point of view, this task will effectively bring NPAC commodity cluster, including a mix of Linux and NT PCs, as one of the HPC resources available for our Metacomputing CMS experiments. By combining the metacomputing aspect and the parallel computing aspect of WebHLA, it will be possible to consider large-scale CMS simulations involving instances of the code running on multiple HPC systems at multiple sites, with each instance being parallel either in a distributed memory fashion via WebHLA or a shared memory fashion via the separate parallel CMS project and past work.

Such a WebHLA based Cluster Management service will be then ported to ERDC and ARL MSRCs to support the Multi-MSRC Metacomputing CMS application running continuously or on-demand in a robust, fault-tolerant, highly-available self-sustained mode.

9. Deliverables:

- WebHLA based cluster management including CF, NF and AF Object Models (June 1999)
- Distributed CMS running on NPAC commodity cluster (September 1999)
- NPAC commodity cluster included into Metacomputing CMS experiments (January 2000)
- Expanding the cluster mgmt tools to metacomputing environment in support of multi-MSRC parallel CMS (March 2000)
- Final Technical Report
- Written progress reports in June and December 1999
- Presentations for PET Mid-Year and Annual Reviews
- Contributions to PET Annual Report

ERDC MSRC PET YEAR 4 EFFORTS

1. **Focused Effort Title:** New Directions in Distance Education and Training
2. **Organization:** Syracuse University, NPAC
3. **Thematic Area(s):** HPC Training and DoD User Productivity
4. **PI Name:** Dr. David Bernholdt
5. **E-Mail Address:** bernhold@npac.syr.edu
6. **Telephone:** 315-443-3857
7. **Fax:** 315-443-1973
8. **Statement of Work:**

In this proposal, we build upon the successes of the last several years to expand both the scope of distance education, and the quality and sophistication of courseware which can be delivered to remote classrooms or training sites. The project includes training/education-specific enhancements for Tango, the development of two new high-quality training modules, and the delivery of a number of courses (both academic and condensed) to JSU, ERDC MSRC, and other sites.

Over the last two years, Syracuse and Jackson State Universities have collaborated, with significant financial and technical support from ERDC MSRC and the PET program, to make distance education a reality. As "spin-offs" from this, JSU faculty are now delivering to other institutions the first course that Syracuse delivered to JSU, and instructors from the Ohio Supercomputer Center have delivered two PET training classes using Tango. Collectively, the experience gained in these efforts has lead to significant improvements in the capability and robustness of the Tango Interactive system itself, and the broader acceptance of distance training with commitments from PET partners for seven training courses to be delivered via Tango in Year 4.

Much of DoD training for the MSRC and university education uses "low-end" approaches such as Powerpoint as this is very suitable for rapidly changing topics. However we believe that it is useful to develop in some areas sophisticated training material where the topics are changing less rapidly. Here we have tentatively identified "basic parallel programming" as an example of core technology worth focusing on. We suggest that it makes sense to develop all new material so that it can both be viewed asynchronously over the web and delivered synchronously using TANGO Interactive. This requires that we establish procedures (best practices) for key authoring techniques and package them for easy use.

In addition to these activities, we plan to promote distance training to others by providing a focused workshop for the faculty of Jackson State University and, upon request, other institutions.

9. Deliverables:

- TANGO Interactive support for glossaries and interactive quizzes (January 2000)
- TANGO Interactive support for embedded applets and Javabeans (November 1999)
- Distance training in basic parallel computing (February 2000 or later, per ERDC MSRC) (beta version of software December 1999)
- Academic credit class using production version of basic parallel computing courseware delivered to JSU and other interested sites (January-March 2000)
- CD-ROM of parallel computing courseware (usable in asynchronous self-study fashion) ready for duplication and distribution at DoD HPC User Group Conference or other appropriate venues (March 2000)
- CPS616 - Web Technologies and Software delivered as academic credit class to JSU and other interested sites (August-December 1999)
- Distance Education Development and Delivery Workshop for JSU faculty (August 1999)
- Contributions to PET Annual Report
- Written progress reports in June and December 1999
- Presentations for PET Mid-Year and Annual Reviews
- Final Technical Report

1. **Focused Effort Title:** Web Interfaces for Computational Modules
2. **Organization:** Syracuse University, NPAC
3. **Thematic Area(s):** HPC Training and DoD User Productivity
4. **PI Name:** Dr. David Bernholdt
5. **E-Mail Address:** bernhold@npac.syr.edu
6. **Telephone:** 315-443-3857
7. **Fax:** 315-443-1973
8. **Statement of Work:**

During the year 3 we have demonstrated feasibility of implementing a system that would allow launching and controlling the complete simulation from a networked laptop. In particular, we successfully implemented a web interface to the LMS, and we are applying this technology to applications of the Mobility System Division.

In spite of the success of the WebFlow project, we see that our current implementation, in which the middle-tier is given by a mesh of Java enhanced Web Servers, suffers from a number of significant limitations. Two the most important areas of improvement are fault tolerance and security. To this end we are re-implementing the WebFlow middle-tier using industry standard distributed object technologies: JavaBeans and CORBA, and industry standard secure communication channels: https (front-end), SSL-based ORB (middle-tier), and GSS-API interface to Keberos5 (secure access to the back-end computational resources).

There is a natural synergy between the proposed work here and the on-going Gateway project at ASC MSRC. The NPAC activities within the Gateway project are focused on delivering the middle-tier solution and its coupling with the high performance resources available at ASC MSRC. The development of the core WebFlow functionality is thus funded outside the PET programs. Within this project we propose to install the upgraded WebFlow at ERDC. This will require customization of interfaces to match the ERDC computational environment.

The main thrust of the proposed work is directed towards building an environment that will allow creation of custom, application specific web-based front-ends interfacing the Gateway middle-tier and transfer this technology directly to application developers at ERDC. We will demonstrate the system using a suite of applications from different CTAs.

9. Deliverables:

- Participation in technical meeting at ERDC on implementation of improved WEBFLOW functionality within computational systems using WEBFLOW at ERDC (July 1999)
- Implementation of the core of the WebFlow system at ERDC (August 1999)
- Initial updates to computational systems at ERDC employing WEBFLOW paradigm (September 1999, December 1999)
- Final release, including improvements based on user feedback, full documentation (March 2000)
- User training at ERDC (March 2000)
- Contributions to PET Annual Report
- Written progress reports in June and December 1999
- Presentations for PET Mid-Year and Annual Reviews
- Final Technical Report

ERDC MSRC PET YEAR 4 EFFORTS

1. **Core Support Area:** SPP Tools, Off-site
2. **Organization:** University of Tennessee, Knoxville
3. **Lead:** Dr. Shirley Browne
4. **E-Mail Address:** browne@cs.utk.edu
5. **Telephone:** 423-974-3547
6. **Fax:** 423-974-8296
7. **Statement of Work:**

   Tennessee will provide core support in the transfer of parallel processing tools to the ERDC MSRC users. These activities include attendance at reviews, planning meetings, and user meetings; reporting; assistance to onsite SPP Tools lead in maintaining and updating PET web pages; assistance to CTAs with use of Repository in a Box (RIB) software; and assistance to onsite SPP Tools lead and CTAs in evaluation, installation, and use of math software and iterative methods. Targeted Codes/Algorithms include ScaLAPACK, Iterative Methods, and Repository in a Box (RIB). UTK will assist with installation of the most recent Netlib version of ScaLAPACK at ERDC MSRC, testing and bug reporting of vendor versions, and consulting on the use of Netlib and vendor versions. Susan Blackford will collaborate with appropriate ERDC MSRC personnel regarding ScaLAPACK issues. Victor Eijkhout has carried out a comprehensive evaluation of available iterative methods software for solution of sparse linear systems. He has also done research, developed software, and published in this area for several years. Dr. Eijkhout will be available on an as-needed basis for consulting in this area. CFD PET is proposing a focused effort to develop a toolkit for engineers to solve sparse linear systems and can contact Dr. Eijkhout for advice if needed. UTK will assist ERDC MSRC staff with installation and maintenance of the most recent version of Repository in a Box (RIB) and will assist CTAs in using RIB to set up repositories. Scott Wells will collaborate with appropriate ERDC MSRC personnel regarding RIB issues.

8. **Deliverables:**

   - Assist onsite SPP Tools lead with installation of Netlib version of ScaLAPACK on ERDC MSRC platforms
   - Provide consulting to CFD CTA and MSRC on iterative solvers
   - Attend and participate in DoD HPC Users meeting
   - Provide assistance with use of new version of Repository in a Box, expected to be released in June 1999
   - Attend ERDC MSRC PET year 4 Annual Review
   - Participation in JSU Summer Institute
   - Written progress reports in June and December 1999
   - Presentations for PET Mid-Year and Annual Reviews

- Contributions to PET Annual Report
- Performance Optimization Training Course

1. **Focused Effort Title:** Parallel I/O for Distributed Applications
2. **Organization:** University of Tennessee, Knoxville
3. **Thematic Area(s):** Scalable Computing Migration, HPC Performance Metrics / Tools
4. **PI Name:** Dr. Graham Fagg
5. **E-Mail Address:** fagg@cs.utk.edu
6. **Telephone:** 423-974-5790
7. **Fax:** 423-974-8296
8. **Statement of Work:**

In this project Tennessee will continue the successful MPI-Connect project that was demonstrated in the ERDC MSRC HPC Challenge at SuperComputing 98, and to allow it to incorporate changes and newer technologies within distributed high-performance computing as they appear.

The proposed work is to cover three areas:
1) Provision of better file handling and management facilities that integrate the newly emerging vendor implementations of MPI-2 parallel IO.
2) Scheduling across sites for multi-machine parallel jobs
3) Integration of features from other metacomputing projects such as Globus

Currently different vendors' MPI implementations cannot interoperate directly with each other. As a result, use of distributed computing across different vendors' machines requires use of a single MPI implementation, such as MPICH. This solution may be sub-optimal because it cannot utilize the vendors' own optimized MPI implementations. MPI-Connect, a software package currently under development at the University of Tennessee, Knoxville, provides the needed interoperability between different vendors' optimized MPI implementations. MPI-Connect is transparent to MPI applications in that it allows intercommunication between different MPI implementations (or instances of the same implementation) using normal MPI communication calls. Additionally, MPI-Connect allows flexible control over MPI applications by providing access to process control and resource control functions.

9. **Deliverables:**

- Continued development and maintenance of MPI_Connect to allow for user requested features and enhancements
- An MPI-2 parallel I/O subsystem that functions across machines (October 1999)
- Set of management tools for handling files spread across multiple machines (December 1999)

- A pre-fetch file system that makes better use of network bandwidth and allows for faster application turn around by moving files closer to computational resources (October 1999)
- MPI_Connect workshop on interconnection technologies and solutions and on file management across multiple domains (January 2000)
- Trip Reports
- Contributions to PET Annual Report
- Presentations for PET Mid-Year and Annual Reviews
- Written progress reports in June and December 1999
- Final Technical Report

ERDC MSRC PET YEAR 4 EFFORTS

1. **Core Support Area:** Environmental Quality Modeling (EQM), On-site and Off-site
2. **Organization:** University of Texas at Austin, TICAM
3. **Lead:** Prof. Mary Wheeler
4. **E-Mail Address:** mfw@ticam.utexas.edu
5. **Telephone:** 512-475-8625
6. **Fax:** 512-471-8694
7. **Statement of Work:**

   In this project Texas will support research and an on-site person in the EQM area; however, it may have applications to other areas, such as CFD. Technology transfer will occur through on-site EQM personnel, EQM web page, activity reporting, and user training. Texas personnel will accomplish user outreach through frequent visits to user sites. Key ERDC MSRC personnel will also be visiting The University of Texas at Austin. Technology transfer will concentrate on the following codes: ADCIRC3D--parallel migration of new 3D baroclinic model; CE-QUAL-ICM and CE-QUAL-ICM/TOXI--provide assistance in mesh partitioning and date I/O; FEMWATER--provide curve fitting algorithms for treating nonlinear media functions, relative permeability and capillary pressure.

8. **Deliverables:**

   - Trip Reports
   - Contributions to PET Annual Report
   - Written progress reports in June and December 1999
   - Presentations for PET Mid-Year and Annual Reviews
   - Workshop on Coupling Multiphysics Problems
   - Workshop on Parallel Algorithms
   - Support to the JSU Summer Institute
   - At least one technical report submitted by on-site lead

1. **Focused Effort Title:** A General Parallel 3D Local Conservative Projection Algorithm
2. **Organization:** University of Texas at Austin, TICAM
3. **Thematic Area(s):** Scalable Computing Migration
4. **PI Name:** Prof. Mary Wheeler and Prof. C.N. Dawson
5. **E-Mail Address:** mfw@ticam.utexas.edu, clint@ticam.utexas.edu
6. **Telephone:** 512-475-8625, 512-475-8627
7. **Fax:** 512-471-8694
8. **Statement of Work:**

   This project is essential to the current EQM efforts in coupling of hydrodynamic codes such as ADCIRC and RMA10 with CE-QUAL-ICM. Software developed here can also be applied to subsurface transport. During Year 4, we propose to develop an efficient parallel domain decomposition solver for the 3D-projection code. In addition, we propose to test this code on realistic 3D and 2D data sets.

   In the numerical modeling of fluid flow and transport problems, the computed velocity field frequently needs to be projected from one grid to another between different models. Usually the flow and multi-species transport are solved separately using completely different numerical methods and grids due to differences in length and time scales of the phenomena involved. For accurate transport, it is necessary for the velocities to be locally conservative on the transport grid. Lack of local mass conservation results in spurious sources and sinks to the transport equation. Local mass conservation can be accomplished through a projection algorithm, which was formulated and analyzed by the investigators.

9. **Deliverables:**

   - Parallel 3D UTPROJ – July 30, 1999
   - Domain Decomposition Solver – November 30, 1999
   - User's manual and training – March 31, 2000
   - Trip reports
   - Contributions to PET Annual Report
   - Written progress reports in June and December 1999
   - Presentations for PET Mid-Year and Annual Reviews
   - Final Technical Report

ERDC MSRC PET YEAR 4 EFFORTS

1. **Focused Effort Title:** Debugging, Validation, and Evolution of Parallel EQM Codes
2. **Organization:** University of Texas at Austin, TICAM
3. **Thematic Area(s):** Scalable Computing Migration
4. **PI Name:** Prof. Mary Wheeler and Dr. Victor Parr
5. **E-Mail Address:** mfw@ticam.utexas.edu, parr@ticam.utexas.edu
6. **Telephone:** 512-475-8625, 409-826-3956
7. **Fax:** 512-471-8694
8. **Statement of Work:**

   The Texas team has helped to parallelize several versions of a number of EQM codes, including CE-QUAL-ICM and ADCIRC. We have also provided extensive consulting in the ongoing parallelization of CE-QUAL-ICM/TOXI. These codes are important components of our efforts in coupling hydrodynamic flow and water quality modeling. More complex physics, chemistry and subsequently more complicated mathematical models are constantly being added to these codes to tackle new applications. These enhancements necessitate modifications/improvements to algorithms, adding of new components/species, new boundary conditions, improved mesh partitioning and handling of data I/O, etc. We propose to continue our collaboration with the software developers and EQM applications personnel in debugging, validating and enhancing the parallel capability and performance of these codes as new versions are being developed.

   Within the next year, new applications of CE-QUAL-ICM are planned, and a new 3D baroclinic version of ADCIRC is under development. As part of this effort, we will investigate the use of the parallel debugging tools developed by the University of Tennessee, Knoxville, PET team, as appropriate.

9. **Deliverables:**

   - Final Technical Report
   - Contributions to PET Annual Report
   - Written progress reports in June and December 1999
   - Trip reports
   - Presentations for PET Mid-Year and Annual Reviews

ERDC MSRC PET YEAR 4 EFFORTS

1. **Core Support Area:** Computational Structural Mechanics (CSM), Off-site
2. **Organization:** University of Texas at Austin, TICAM
3. **Lead:** Prof. Tinsley Oden
4. **E-Mail Address:** oden@ticam.utexas.edu
5. **Telephone:** 512-471-3312
6. **Fax:** 512-471-8694
7. **Statement of Work:**

   TICAM will provide a core level of effort to support technology transfer, user outreach, and training. Technology of interest includes, but is not limited to, adaptive mesh and grid algorithms and tools, management of large CSM data sets, and parallelization/coupling of key CSM codes. Texas will maintain regular contact with the ERDC MSRC PET On-Site Lead for CSM to facilitate technology transfer, user outreach, and relevance to current MSRC issues. Related codes include CTH, EPIC and DYNA3D. During the year, TICAM will make site visits to ERDC MSRC to work with the DoD users and on-site personnel for CSM.

   TICAM will select and attend focused conferences and other meetings that have high payoff and direct application for user interaction and technology transfer. Targeted training includes, but is not limited to, training courses/workshops on grid generation, adaptive grids, management of large data sets, and efficient reliable HPC computations. Such training may be conducted either at ERDC MSRC or at remote user sites as deemed necessary and appropriate. TICAM will work with the On-site Team Lead to arrange training classes during the year.

8. **Deliverables:**

   - One or more papers or poster sessions will be submitted for presentation at the next DoD HPC Users Group Meeting
   - Trip reports for conferences and user contacts (as conducted)
   - Contributions to PET Annual Report
   - Presentations for PET Mid-Year and Annual Reviews
   - Contributions to CSM portion of ERDC MSRC PET website
   - Written progress reports in June and December 1999
   - Grid Training Course
   - Adaptive Training Course
   - Support for JSU Summer Institute

ERDC MSRC PET YEAR 4 EFFORTS

1. **Focused Effort Title:** Adaptive Mesh Technology Applied to Damaged Structures
2. **Organization:** University of Texas at Austin, TICAM
3. **Thematic Area(s):** Scalable Computing Migration
4. **PI Name:** Prof. Graham Carey and Prof. Tinsley Oden
5. **E-Mail Address:** carey@cfdlab.ae.utexas.edu**,** oden@ticam.utexas.edu
6. **Telephone:** 512-471-4676 (Carey), 512-471-3312 (Oden)
7. **Fax:** 512-232-3357 (Carey), 512-471-8694 (Oden)
8. **Statement of Work:**

   TICAM will promote and develop unstructured grid approaches and adaptive grid technology that will enhance the accuracy and performance of Computational Structural Mechanics (CSM) codes used by DoD researchers for Damaged Structures Analysis. This project involves issues related to compatibility of existing data structures in current DoD analysis codes to handle unstructured grids, mesh refinement or coarsening and remeshing. It also deals with problems related to application programming interfaces to meet the adaptive mesh refinement (AMR) objective, support of AMR data structures, development of *a posteriori* error estimates and computable error indicators to guide mesh refinement assessment and improvement of grid geometric quality and development and testing of software modules for error indicator and reliability calculations. This effort will concentrate on CTH block refinement.

9. **Deliverables:**

   - Contributions to PET Annual Report
   - Presentations for PET Mid-Year and Annual Reviews
   - Final Technical Report
   - Contributions to the PET CSM web page on adaptive algorithms, test problems, error analysis, etc.
   - Technical reports and journal articles detailing results of the project, new algorithm development and error indicator/adaptivity analysis
   - Software for CSM testbed with supporting technical documentation
   - Visit to Vicksburg and briefing to ERDC MSRC on research progress (October 1999)

ERDC MSRC PET YEAR 4 EFFORTS

1. **Focused Effort Title**: Adaptive Mesh Technology For Hypervelocity Impact And Penetration Analyses

2. **Organization:** University of Texas at Austin, TICAM

3. **Thematic Area(s):** Scalable Computing Migration

4. **PI Names**: Prof. Graham Carey and Prof. Tinsley Oden

5. **Email Address**: carey@cfdlab.ae.utexas.edu, oden@ticam.utexas.edu

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7. **Fax:** (512) 232-3357 (Carey) (512) 471-8694 (Oden)

8. **Statement of Work:**

   TICAM will promote and develop unstructured grid approaches and adaptive mesh refinement methods for Computational Structural Mechanics codes used by DoD researchers in hypervelocity impact and penetration analyses. TICAM will develop local mesh refinement strategies for CTH and EPIC type codes and investigate data structure issues related to implementation of various refinement strategies. Local error indicators of residual and recovery types will be formulated and analyzed. A computational testbed will be developed to enable rapid evaluation of indicators and algorithms for very large codes such as CTH. A series of benchmark tests and comparison studies using different error indicators will be performed using the EPIC code. The final task in this focused effort will be to investigate techniques for solving mesh aspect ratio degeneracy and conduct mesh partitioning studies with CTH using TICAM and Sandia code modules.

9. **Deliverables:**

   - Contributions to PET Annual Report
   - Presentations for PET Mid-Year and Annual Reviews
   - Written progress reports in June and December 1999
   - Final Technical Report
   - Presentations at DoD Users Group Meeting
   - Technical reports and journal articles detailing results of the project, new algorithms developed, and error indicator/adaptivity analysis
   - Support for implementation of selected adaption methods in DoD codes
   - Software for the CSM testbed with supporting technical documentation
   - Visit to Vicksburg and briefing to ERDC MSRC on research program (October 1999)

Section 3: Contact Information

3.1 ACADEMIC POINTS OF CONTACT

- Academic Team Lead - Prof. Joe Thompson (ERC - Mississippi State)
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- Training Lead - Prof. Geoffrey Fox (NPAC-Syracuse)
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- CSM Lead - Prof. Tinsley Oden (TICAM-Texas)
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- CWO Lead - Prof. Keith Bedford (Ohio State)
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- SPP Tools Lead - Dr. Richard Hanson (CRPC - Rice)
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- Scientific Visualization Lead - Dr. Polly Baker (NCSA - Illinois)
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3.2 ON-SITE POINTS OF CONTACT

- Government PET Lead - Dr. Louis Turcotte (CEWES MSRC)
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- PET Director - Dr. Henry Gabb (Nichols Research)
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- CFD On-Site Lead - open

- CSM On-Site Lead - Dr. Richard Weed (ERC - Mississippi State)
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- Training Coordinator - Mr. John Eberle (Nichols Research)
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3.3 IMPORTANT WEB ADDRESSES

ERDC Home Page: http://www.erdc.usace.army.mil/

ERDC MSRC Home Page: http://www.wes.hpc.mil/

ERDC MSRC Technical Reports: http://www.wes.hpc.mil/CEWES/reports/index.html

ERDC MSRC PET Training Schedule: http://www.wes.hpc.mil/msrc/training/f_cewes.html

DoD HPCMP Home Page: http://www.hpcmo.hpc.mil/

DoD HPCMP PET Executive Committee: http://www.crpc.rice.edu/DODmod/index.html